Use of Adjoint Physics for 4D VAR with the NCEP Global Spectral Model

Presentation for Ph.D. Dissertation

by

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What is variational analysis?

What is 4D VAR? What good is it?

- Variational analysis: vary control parameters to adjust system to optimal state.

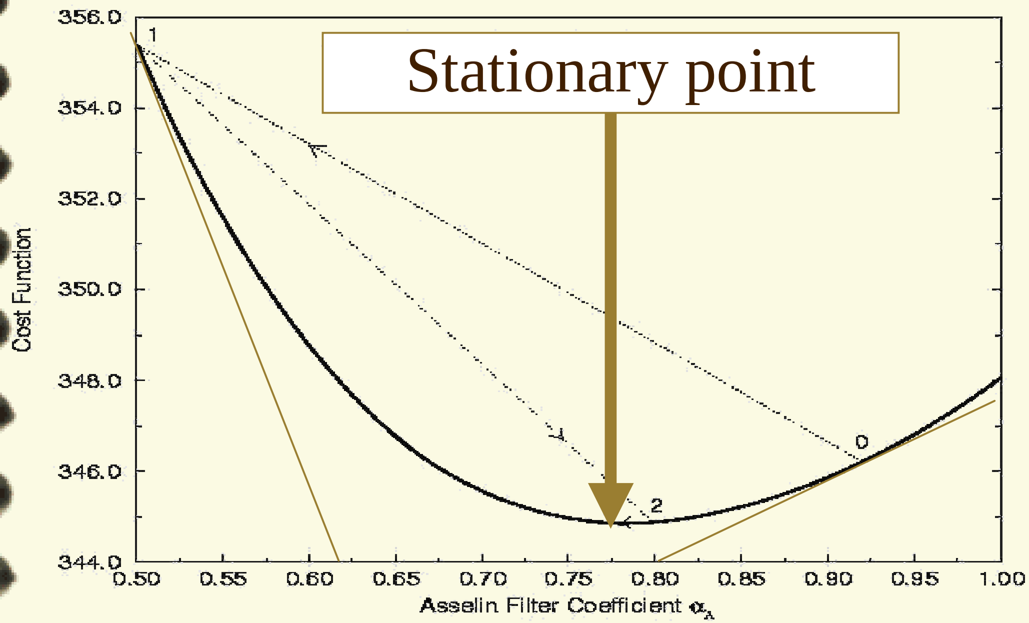
  Control system: NWP model

  Control parameters: ICs, physical parameters

  Optimal state: Minimal forecast errors (cost function).

- 4D VAR: apply variational analysis to minimize a defined cost function over space and time.
- Application: Find an optimal estimate of ICs or parameters, which is internally consistent between model dynamics and observations.

What are minimization and adjoint?



- ✓ A minimization algorithm seeks a stationary point: evaluate cost function and its gradient
- ✓ An adjoint integration efficiently evaluates cost function gradient.

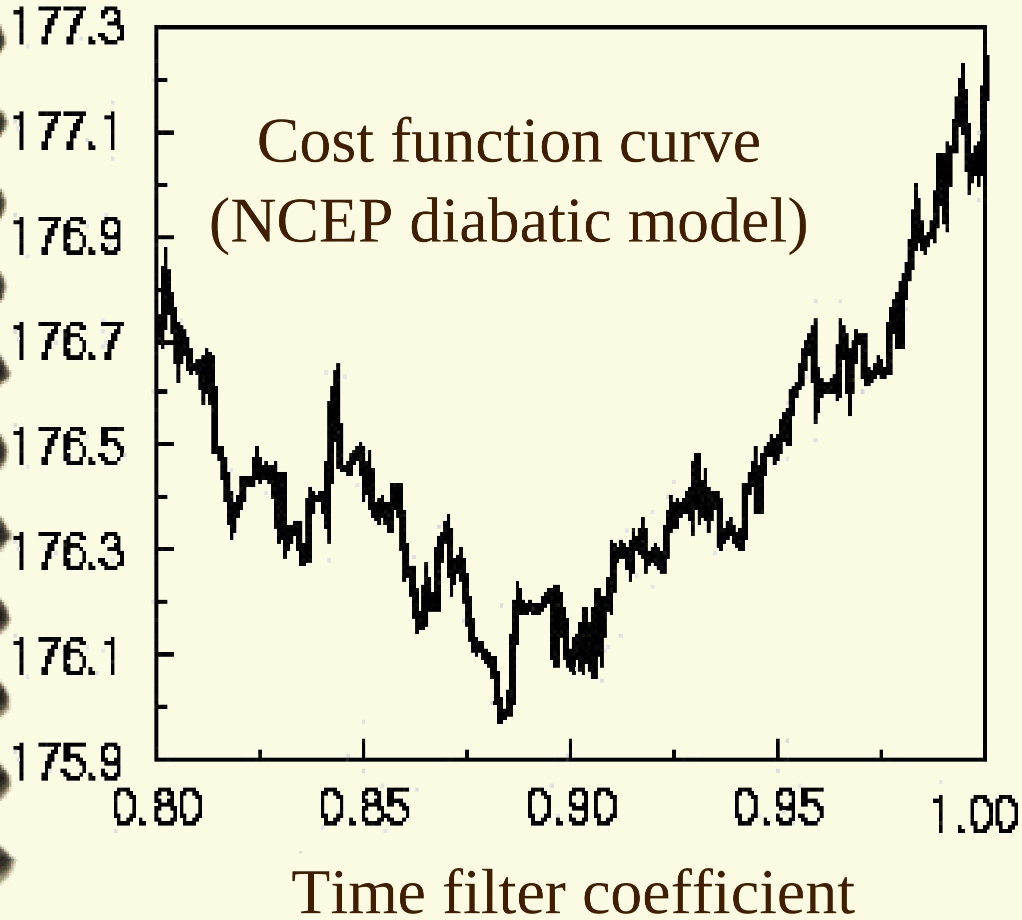
Adjoint sensitivity analysis

ICs & parameters

Error (cost ftn)

Nonlinear Forecast

Challenge: Discontinuous physics



- ✓ Discontinuous physics ⇒ discontinuous cost function.
- ✓ Past approach: smooth discontinuities in physics.
- ✓ Smoothing introduces many additional local minima.

Goals of my research

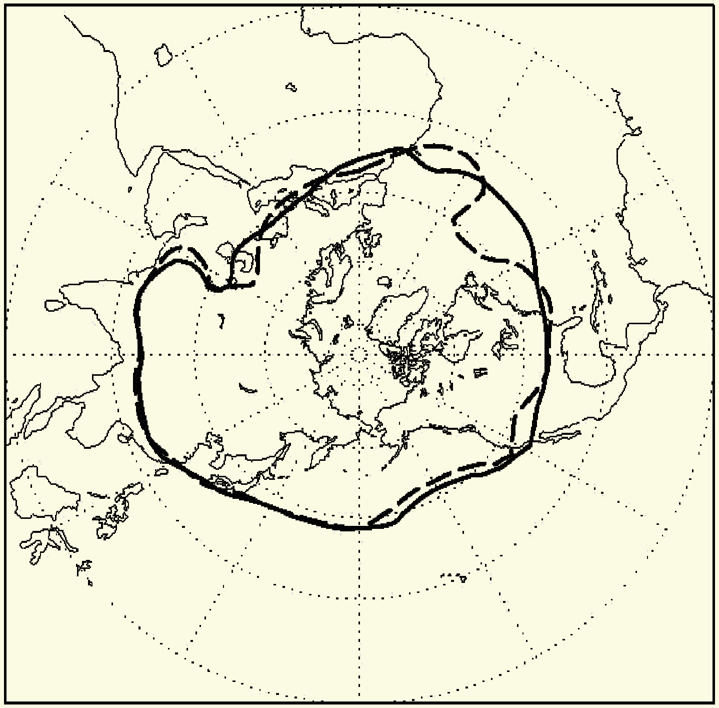
- ✓ Answer questions:
  - – Can an adjoint correctly evaluate the cost function gradient when model physics are discontinuous?
  - – Can a minimization algorithm designed for differentiable functions work for a discontinuous cost function? Do we have a better solution?
- ✓ Construct a variational analysis system with the NCEP global spectral diabatic model
- ✓ Carry out experiments on data assimilation and parameter fitting by 4D VAR approach.

Outline

- ✓ Review of classical approach to variational analysis
  - Lagrange multiplier solves a constrained problem (Sasaki 1958)
  - Optimal control theory (LeDimet & Talagrand 1986)
  - Perturbation analysis (PA) approach to derive the gradient of the cost function (J)
  - Newton and quasi-Newton minimization algorithms.
- ✓ Answers for problems introduced by physics
  - New insight (rather than using PA) between adjoint and gradient:

    Adjoint of discon. physics does work for deriving the gradient of J.
  - Limited Memory Quasi-Newton method (L-BFGS) usually works for minimizing J on discon. physics but sometimes has problems.
  - Bundle method for discontinuous functions is better but slow.
  - Optimal ICs and parameters improve forecasts just for 3 days.
- ✓ Future work

Optimal control problem

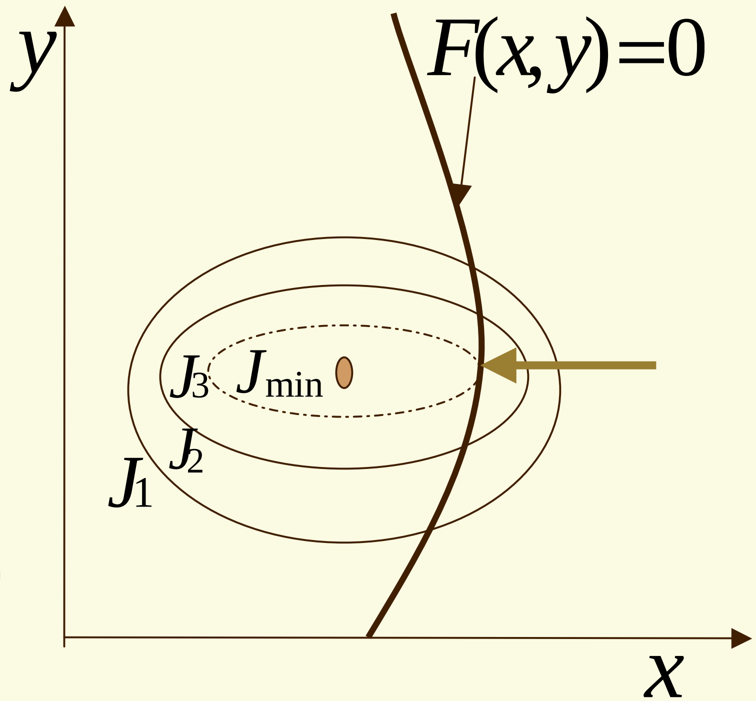


Example: Forecast (solid), observation (dashed)

- Let **x** =column vector of all model variables

  Let **β** =column vector of model parameters
- Let $\frac{\partial \mathbf{x}}{\partial \mathbf{t}} = \mathbf{F}(\mathbf{x}, \boldsymbol{\beta})$ =NWP model
- ***F(x ,β) is discontinuous when parameterized physics are included***
- Let J(**x**) = specified error measurement in a time window (cost function)
- Problem: Find **x** at t=0 and **β** that minimize J

Sasaki (1958): Lagrange multiplier method for constrained problem



- ✓ Lagrange multiplier method constructs a new expression, Lagrangian,

$$L = J(\mathbf{x}) + \boldsymbol{\lambda}^T \mathbf{F}(\mathbf{x})$$

- ✓ Seek the stationary point $(\mathbf{x}, \boldsymbol{\lambda})$ of the Lagrangian by solving Euler-Lagrange equations

$$\begin{cases} \frac{\partial L}{\partial \mathbf{x}} = 0 \\ \frac{\partial L}{\partial \boldsymbol{\lambda}} = 0 \end{cases}$$

But:

- Too many equations
- Poor convergence
- Too expensive computationally

Le Dimet & Talagrand (1986): Adjoint technique to derive gradient by PA

- ✓ Cost function depends on control variable, $\boldsymbol{\alpha}=(\mathbf{x_0},\boldsymbol{\beta})$, with numerical model as bridge:

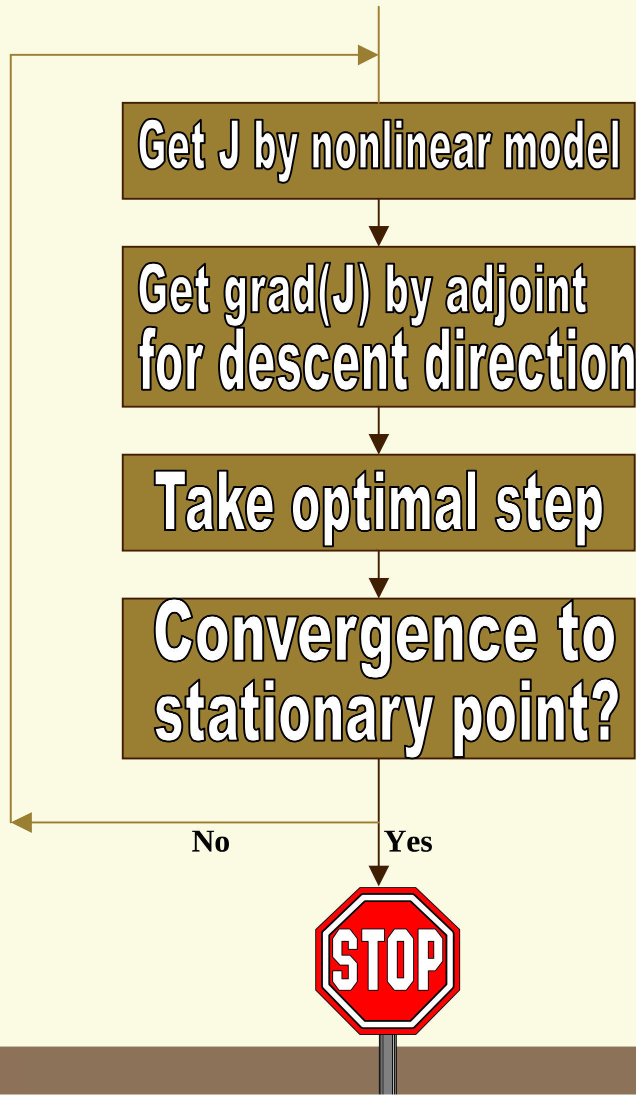
$$\begin{cases} J(\boldsymbol{\alpha}) = \frac{1}{2} < \mathbf{W}(\mathbf{x}-\mathbf{x}^o), (\mathbf{x}-\mathbf{x}^o) > \\ \mathbf{x} = \mathbf{H}\ (\ \boldsymbol{\alpha}\ ) \rightarrow \delta\mathbf{x} = \mathbf{L}\delta\boldsymbol{\alpha} \end{cases} \rightarrow \begin{cases} \delta J = < \mathbf{W}(\mathbf{x}-\mathbf{x}^o), \delta\mathbf{x} > \\ \delta J \overset{\downarrow}{=} < \mathbf{W}(\mathbf{x}-\mathbf{x}^o), \mathbf{L}\delta\boldsymbol{\alpha} > \\ \delta J \overset{\downarrow}{=} < \mathbf{L}^*\mathbf{W}(\mathbf{x}-\mathbf{x}^o), \delta\boldsymbol{\alpha} > \end{cases}$$

- ✓ Since $\delta J = <\nabla|_{\alpha} J, \delta\, \boldsymbol{\alpha}>$, $\nabla|_{\alpha} J = L^* W (\mathbf{x} - \mathbf{x}_0)$, where

  L^* = adjoint of matrix L

- ✓ With the gradient, a minimization algorithm (popularly L-BFGS) can iterate to solve for optimal values of control variables

Newton and quasi-Newton minimization algorithms



- Solve Newton zero roots as an optimal step size (Newton method)

$$J(\boldsymbol{\alpha})=J(\boldsymbol{\alpha}_0)+\nabla_{\alpha} J|_{\alpha_0}(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)+\frac{1}{2}(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)^T\mathbf{A}\,(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)$$

$$\downarrow$$

$$\nabla_{\alpha} J|_{\alpha}=\nabla_{\alpha} J|_{\alpha_0}+\mathbf{A}(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)$$

$$\downarrow$$

$$\nabla_{\alpha} J|_{\alpha_0}+\mathbf{A}(\boldsymbol{\alpha}-\boldsymbol{\alpha}_0)=0$$

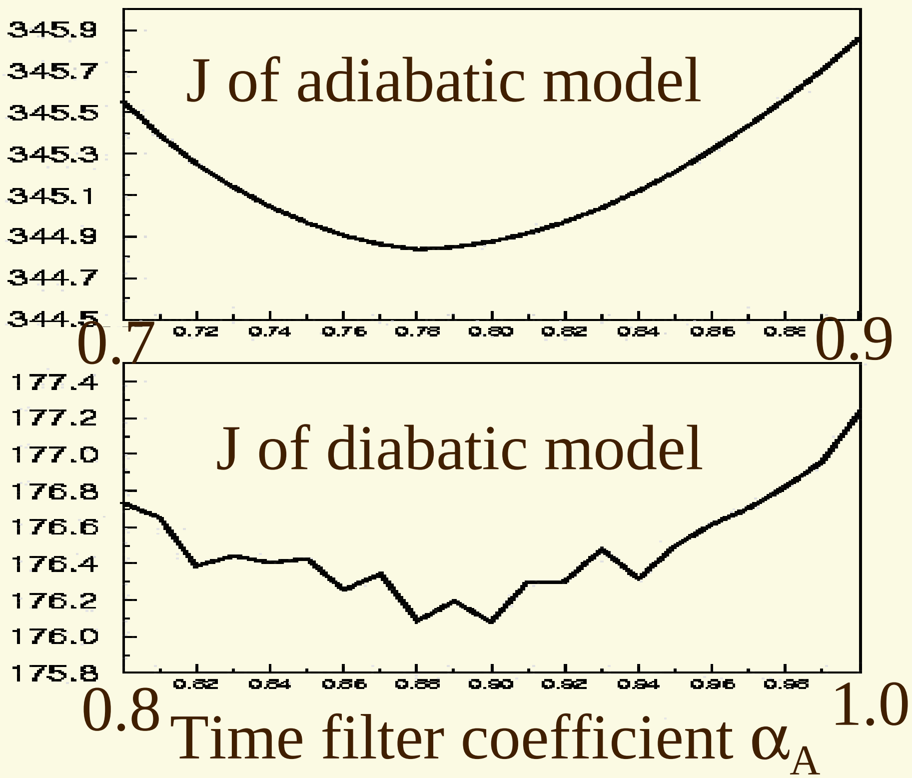
- Iteratively refine the approximation for the inverse of Hessian matrix (quasi-Newton method, L-BFGS)

$$\begin{cases} \mathbf{H}_{n+1}=\mathbf{H}_n+\textbf{correction} \\ \boldsymbol{\alpha}_{n+1}-\boldsymbol{\alpha}_n=\mathbf{H}_{n+1}(\nabla J_{n+1}-\nabla J_n) \\ \lim\limits_{n\to\infty}\mathbf{H}_n=\mathbf{A}^{-1} \end{cases}$$

- Line search to determine optimal stepsize $\beta^{(k)}$

Steps to develop adjoint

- ✓ Code and test TLM: compare $\mathbf{x}(\alpha+\delta\alpha)-\mathbf{x}(\alpha)$ and $\mathbf{L}\ \delta\alpha$
- ✓ Code and test adjoint: compare $J(\alpha+\delta\alpha)-J(\alpha)$ and $\mathrm{grad}(J)\ \delta\alpha$
- ✓ TLM and adjoint tests by PA fail with discont. physics



Ex: Asselin Filter:

$$\tilde{A}(t)=\tilde{A}(t-1)+\varepsilon[\tilde{A}(t-1)-2A(t)+A(t+1)]$$

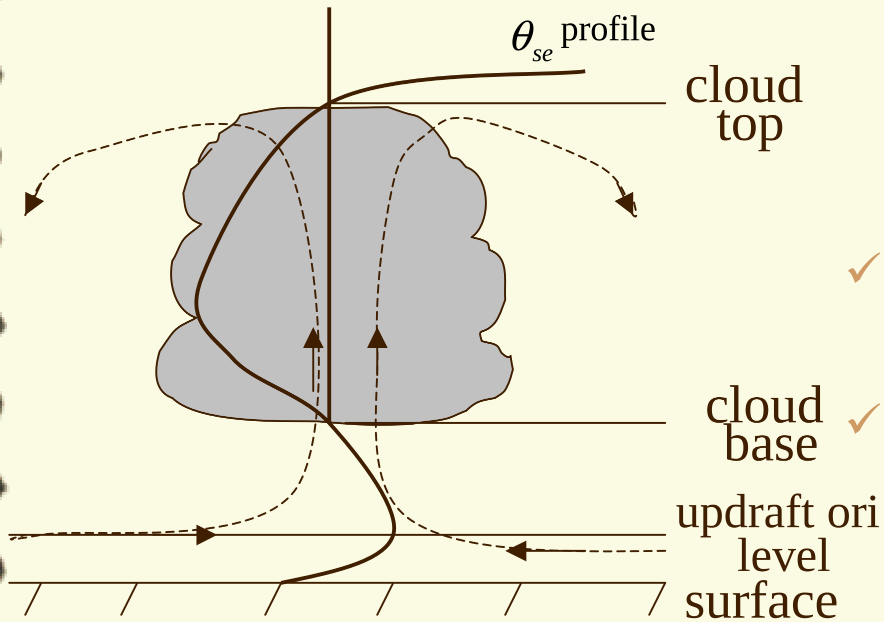
$$\begin{cases} \alpha_A = 1-2\varepsilon \\ \alpha_A = \alpha_{A0} + \Delta\alpha_A \times n \\ \Delta\alpha_A = 0.01 \end{cases}$$

TLM test and gradient test of adjoint based on perturbation analysis

- ✓ Compute $\{\mathbf{x}(\alpha+\beta\delta\alpha) - \mathbf{x}(\alpha)\} / \mathbf{L}\,\beta\delta\alpha$
- ✓ Compute $\{J(\alpha+\beta\delta\alpha) - J(\alpha)\} / \mathrm{grad}(J)\,\beta\delta\alpha$

TLM test			Gradient test of adjoint		
$\log\beta$	ADB-model	DB-model	$\log\beta$	ADB - Model	DB - Model
-1	0.99998	4173.94	-8	1.06577	2.24501
-2	0.99999	12.0942	-9	1.00622	0.25756
-3	1.00000	1.00045	-10	1.00063	-4.1876
-4	1.00000	1.00017	-11	1.00006	1.00129
-5	1.00000	—	-12	1.00000	1.00392
-6	1.00000	1.00031	-13	0.99998	1.00076
-7	1.00000	1.00066	-14	1.00076	0.99967
-8	1.00000	—	-15	0.99849	0.98182
-9	1.00000	—	-16	0.98786	0.81740

Example of discontinuities in a simplified Arakawa-Schubert cumulus parameterization



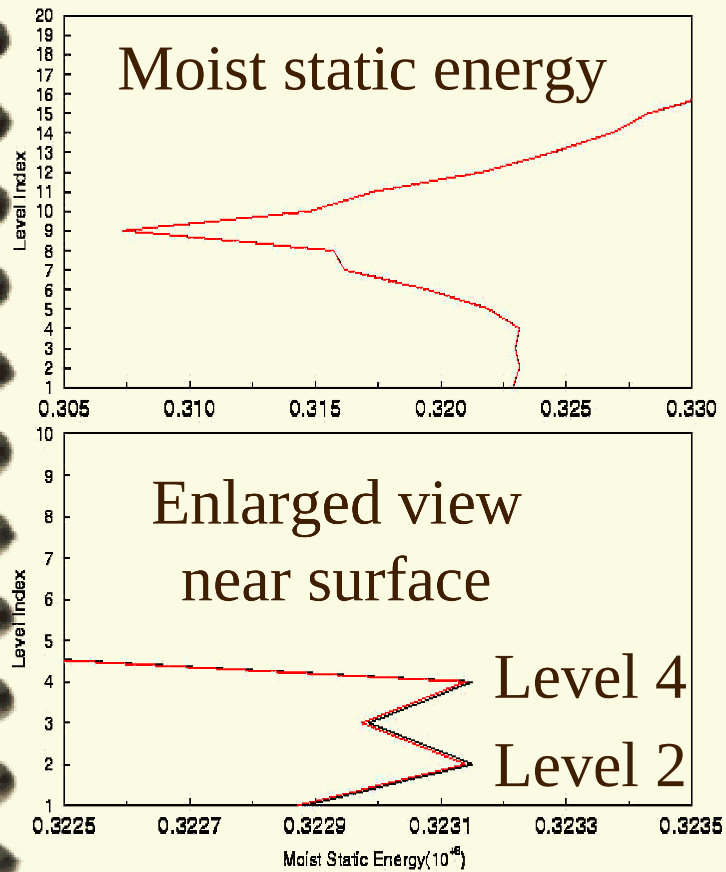
A-S schematic diagram for one cloud type

- Conditional instability defines updraft originating level; cloud base at lifting condensation level; cloud top where parcel θ_{se} equals environment θ_{se}
- 150 hPa is threshold for updraft layer and cloud thickness
- Check diabatic model behavior

  $\mathbf{x}(\alpha+\delta\alpha) - \mathbf{x}(\alpha)$ for initial field on

  1 Nov 1995
- Choose column where initial cumulus is turned off after small change in θ_{se} profile

Example of discontinuities in a simplified Arakawa-Schubert cumulus parameterization

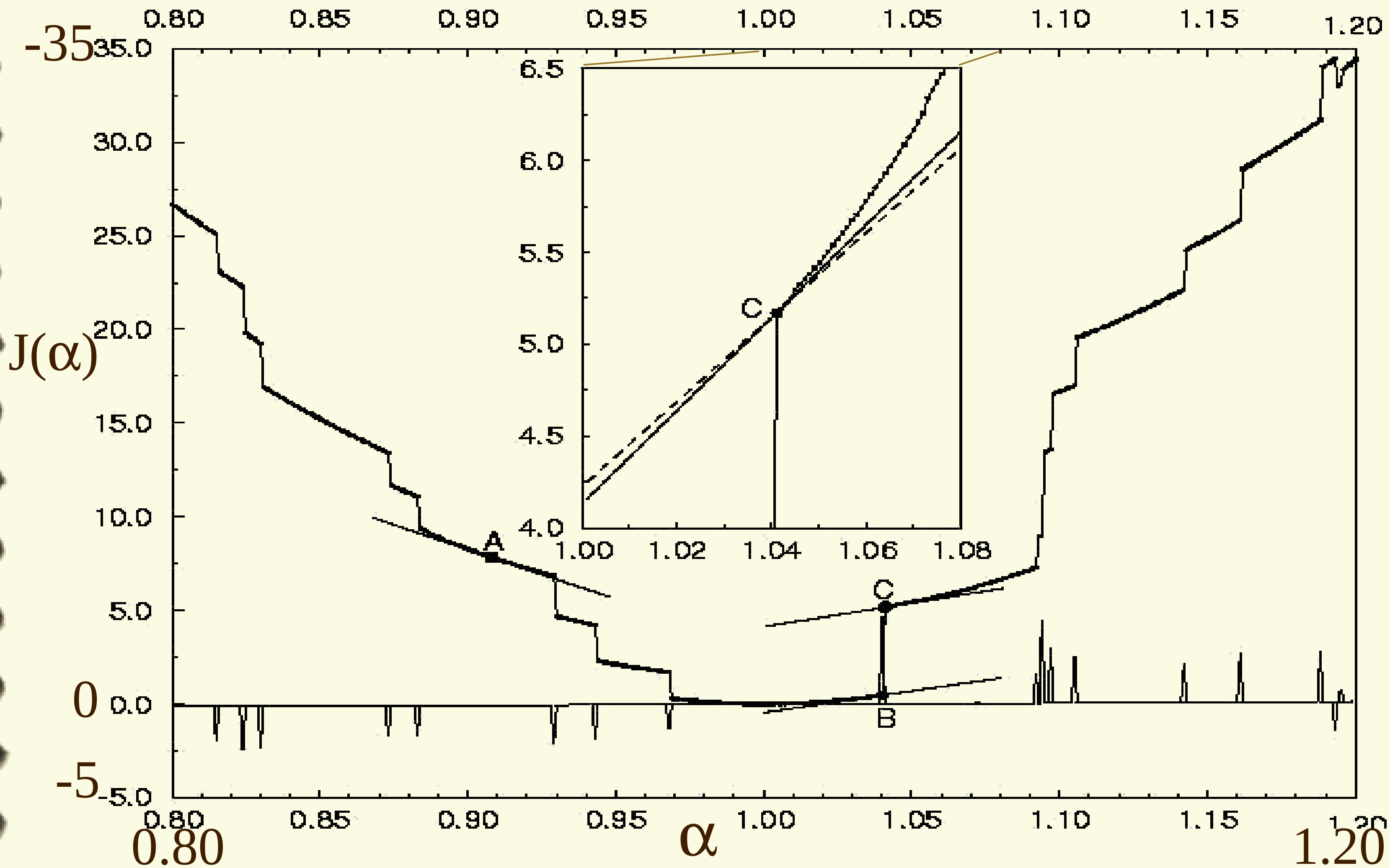


- ✓ Example: column 212, latitude circle 39, time step 3
- ✓ Updraft depth: 154 hPa when level 2 is the updraft originating level; 68 hPa for level 4
- ✓ Any small perturbation may cause cumulus to be turned on/off suddenly
- ✓ Model response jumps

$J(\alpha)=\sum w[f(T,q)-f^{obs}]^2$, f = Arakawa-Sch. parameterization

$T=T_{3.75^oN}+\alpha(T_{1.875^oN}-T_{3.75^oN})$ (28 levels ×384 columns)

by $\alpha=0.8+0.001\times n$ and $f^{obs}=f(T_{1.875^oN},\ q_{1.875^oN})$ on 11/01/95



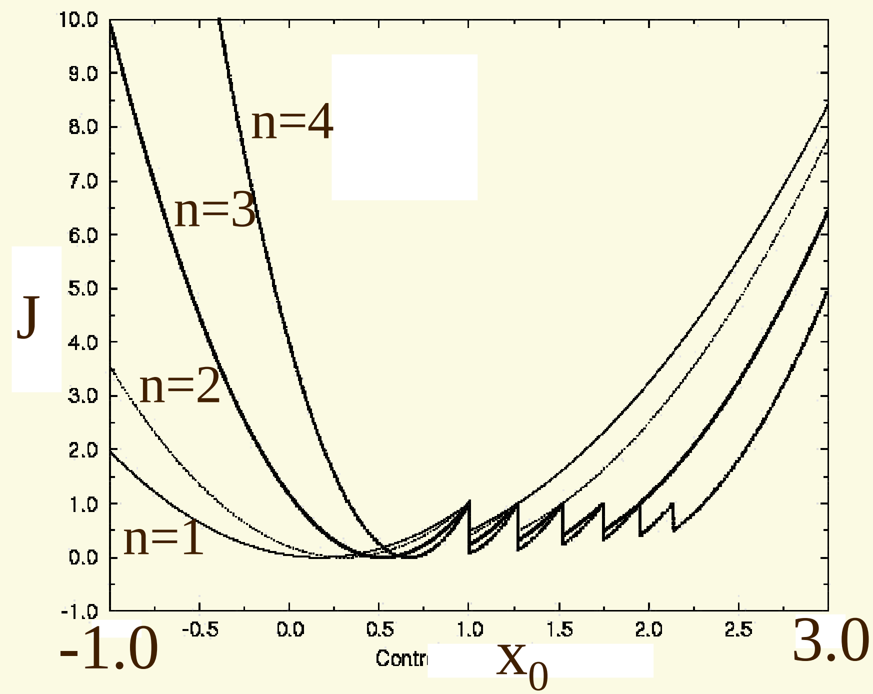
Character of cost function with discontinuous physics: Simple model

- ✓ The cost function, J, is piecewise differentiable due to piecewise differentiable source term (physics).
- ✓ For k thresholds and n time steps, max number of differentiable segments of J is $k \cdot 2^n$

$$\frac{\partial x}{\partial t} = \begin{cases} f_1(x), & x < x_c \\ f_2(x), & x \geq x_c \end{cases}$$

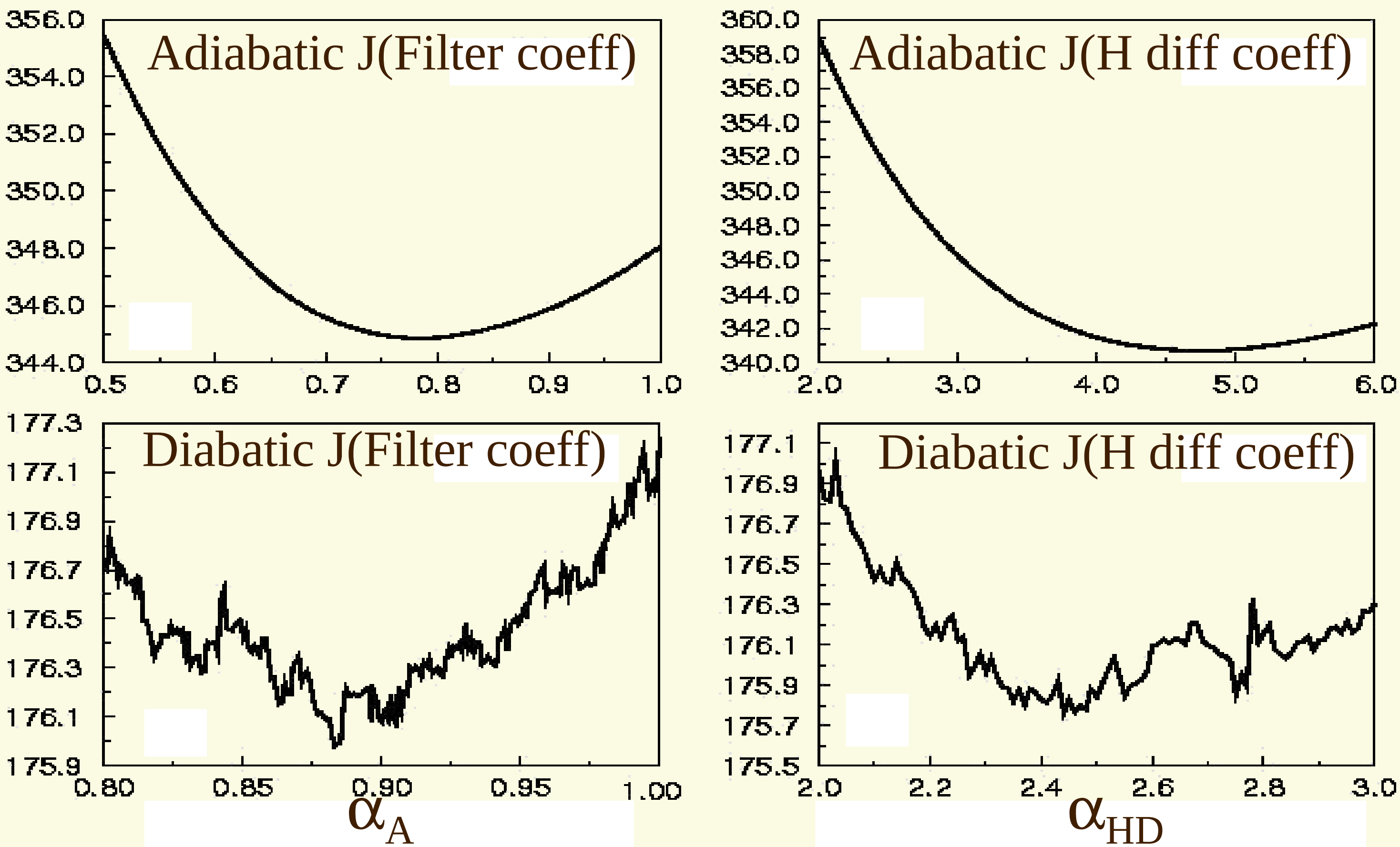
$f_1(x) = 2x-2$, $f_2(x) = x-4$,
$x_c = 1$, $dt = 0.1$.

Cost function:
$J = x^2(t_n)$



Character of cost function with discontinuous physics: Real model

- ✓ A real numerical model is an extension of the single-variable model on grids and variables



Can adjoint of discontinuous physics find cost function gradient? Theory:

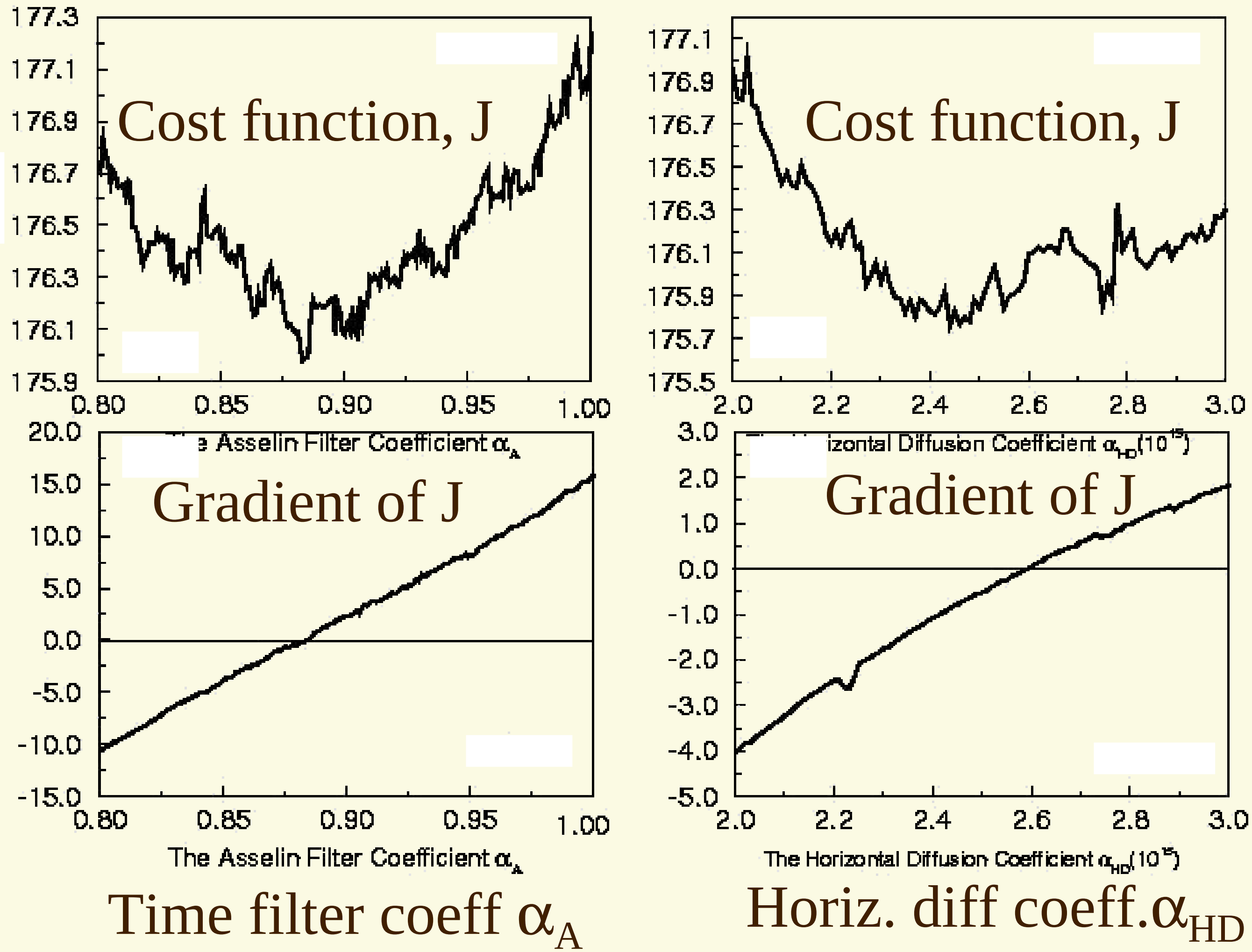
- ✓ Gradient of J of a single-variable model w.r.t. IC is evaluated by chain rule of differentiation, and every integration time step forms a sub-function:

$$\frac{dJ}{dx_0}=\frac{dJ}{dx_n}\frac{dx_n}{dx_{n-1}}\cdots\frac{dx_2}{dx_1}\frac{dx_1}{dx_0}=\left(\frac{dx_1}{dx_0}\frac{dx_2}{dx_1}\cdots\frac{dx_n}{dx_{n-1}}\right)\frac{dJ}{dx_n}\ \text{=adjoint integration of}\ \frac{dJ}{dx_n}$$

- ✓ For multi-variable models, expanding the chain rule forms the integration of an adjoint model:

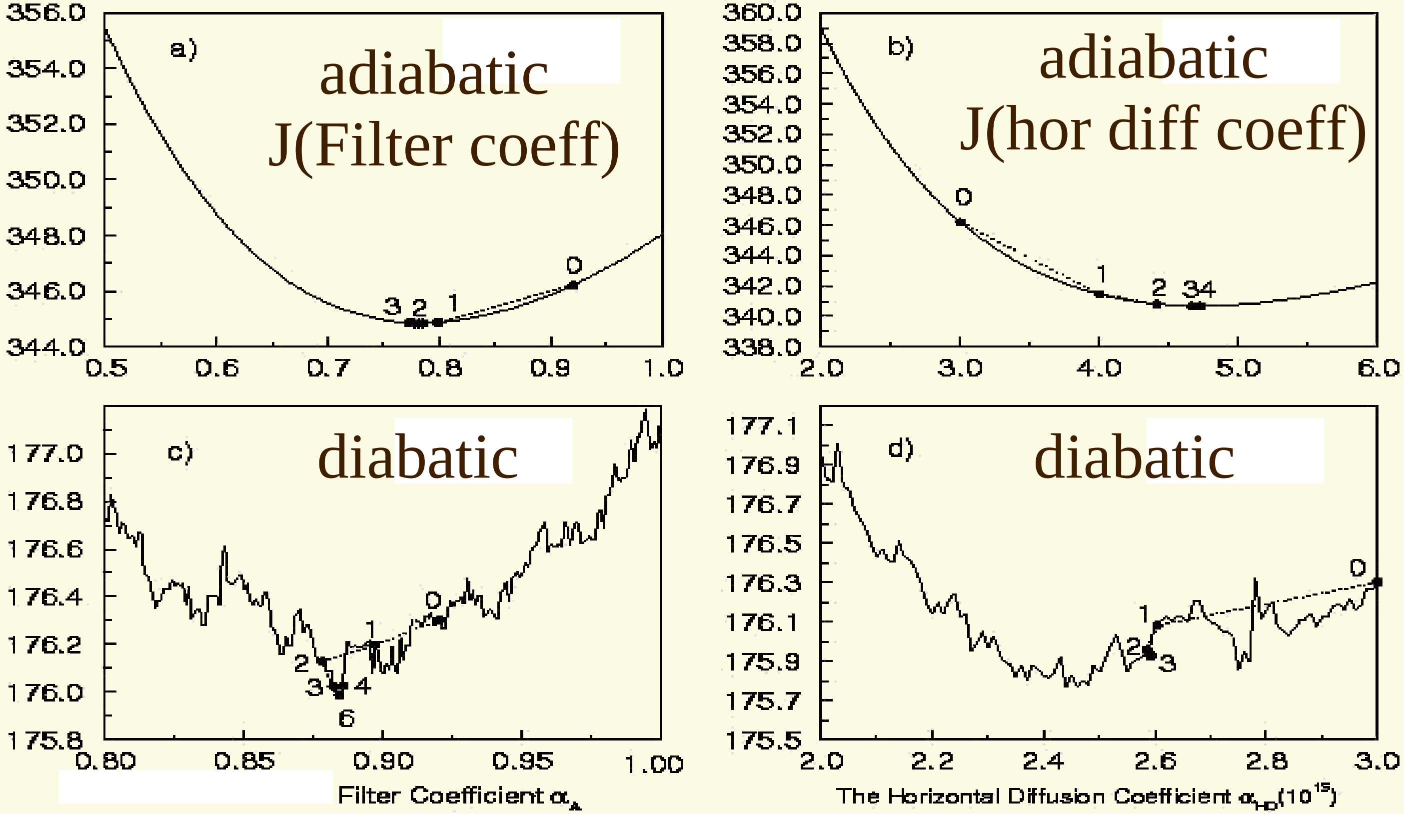
$$\nabla|_{\mathbf{x}_0}J=\begin{pmatrix}\frac{\partial J}{\partial x_{01}}\\ \frac{\partial J}{\partial x_{02}}\\ \vdots\\ \frac{\partial J}{\partial x_{0n}}\end{pmatrix}=\begin{pmatrix}\frac{\partial J}{\partial x_1}\frac{\partial x_1}{\partial x_{01}}+\frac{\partial J}{\partial x_2}\frac{\partial x_2}{\partial x_{01}}+\cdots+\frac{\partial J}{\partial x_n}\frac{\partial x_n}{\partial x_{0n}}\\ \frac{\partial J}{\partial x_1}\frac{\partial x_1}{\partial x_{02}}+\frac{\partial J}{\partial x_2}\frac{\partial x_2}{\partial x_{02}}+\cdots+\frac{\partial J}{\partial x_n}\frac{\partial x_n}{\partial x_{02}}\\ \vdots\\ \frac{\partial J}{\partial x_1}\frac{\partial x_1}{\partial x_{0n}}+\frac{\partial J}{\partial x_2}\frac{\partial x_2}{\partial x_{0n}}+\cdots+\frac{\partial J}{\partial x_n}\frac{\partial x_n}{\partial x_{0n}}\end{pmatrix}=\mathbf{L}_1^T\mathbf{L}_2^T\cdots\mathbf{L}_{t_R}^T\frac{\partial J}{\partial \mathbf{x}}=\mathrm{L}^{\mathrm{T}}\frac{\partial \mathrm{J}}{\partial \mathrm{x}}$$

Can adjoint of discontinuous physics find cost function gradient? Yes.



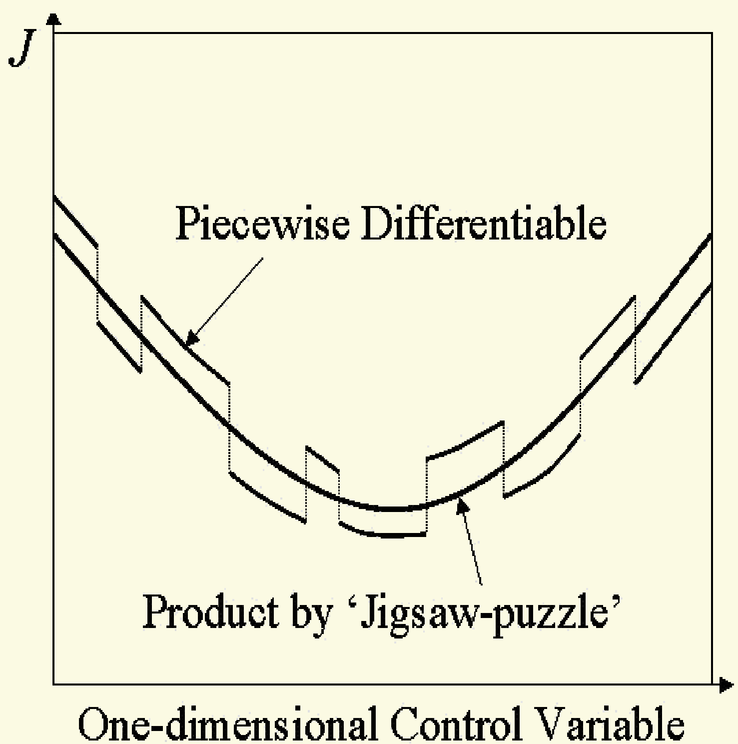
Can quasi-Newton algorithm minimize a piecewise differentiable J? Often yes.

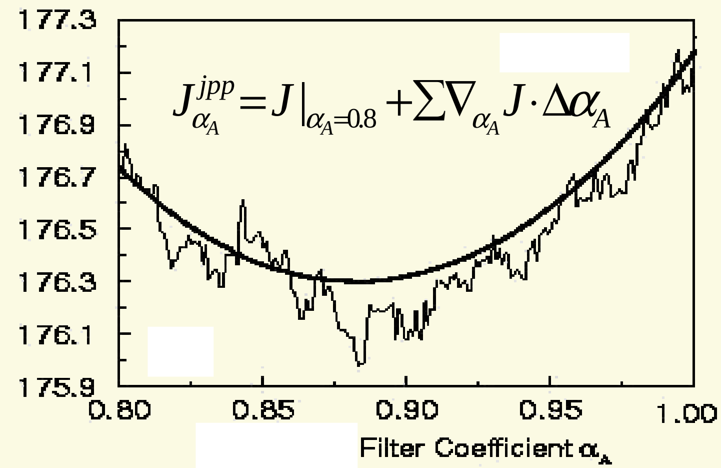
- ✓ L-BFGS algorithm can usually find the stationary point of J with the correct gradient evaluated from the adjoint.
- ✓ The stationary point may not be the global minimum.

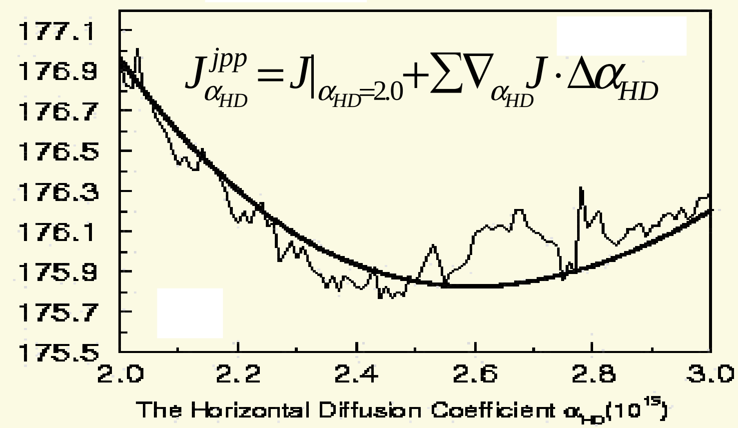


Can quasi-Newton algorithm minimize a piecewise differentiable J? Often yes.

- ✓ Rough curve = actual cost function
- ✓ Smooth curve = integral of gradient. Similar minima.







L-BFGS algorithm (quasi-Newton) minimizes piecewise differentiable J for 282 of 300 ICs.

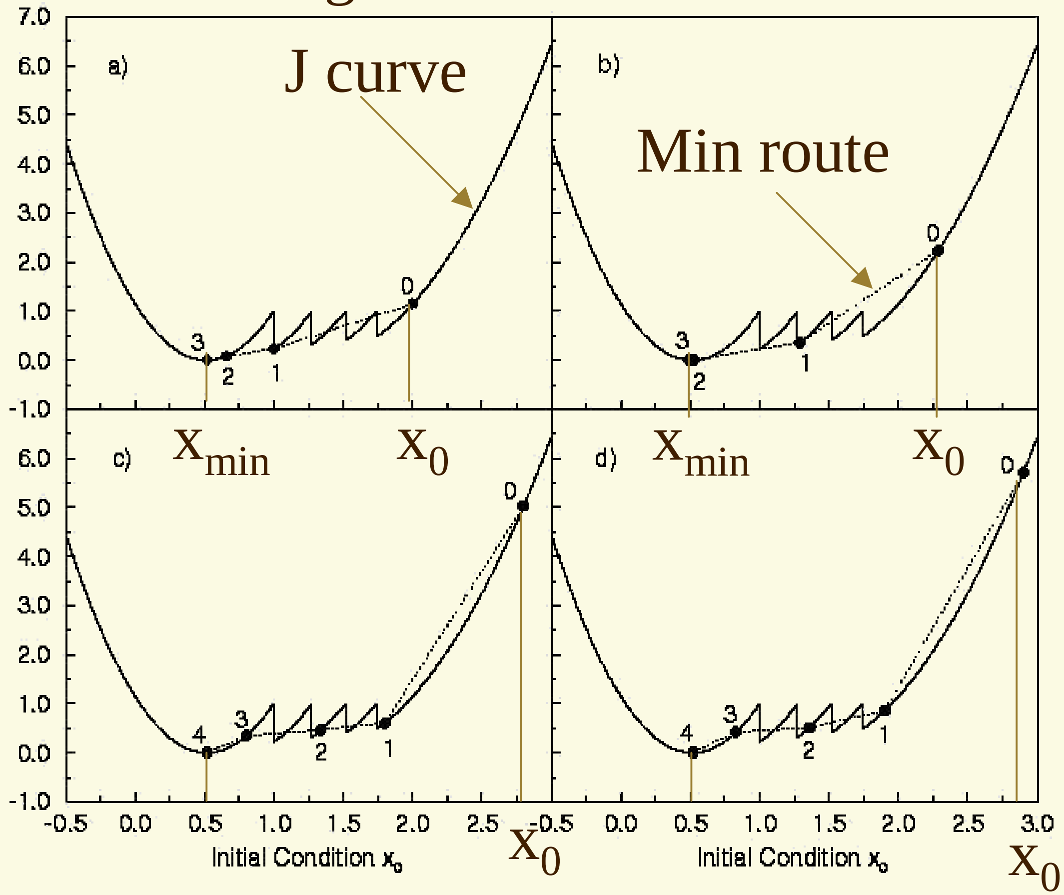
Test case:

$$\frac{\partial x}{\partial t} = \begin{cases} 2x - 2, & x < 1 \\ x - 4, & x \geq 1 \end{cases}$$

Integrate forward
4 steps with dt = 0.1

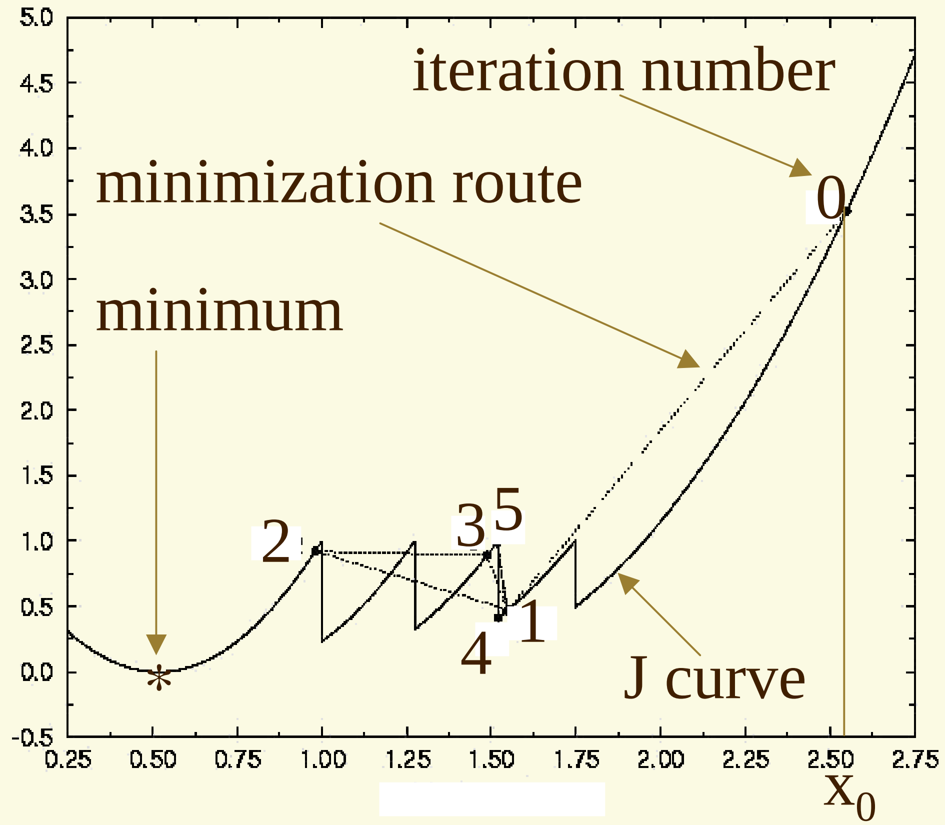
Cost function:
J = x^2 at t_4

Successful minimization of J starting from 4 different ICs



One example from the 18 failed cases: Same equations, different initial guess for x_0

- ✓ Minimization trapped by discontinuity
- ✓ Algorithm works if jump size reduced.

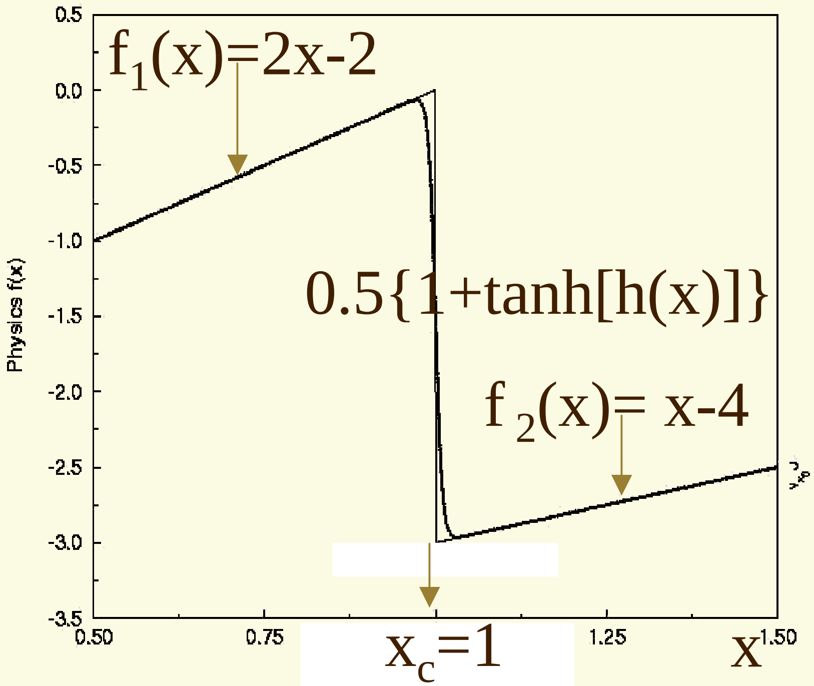


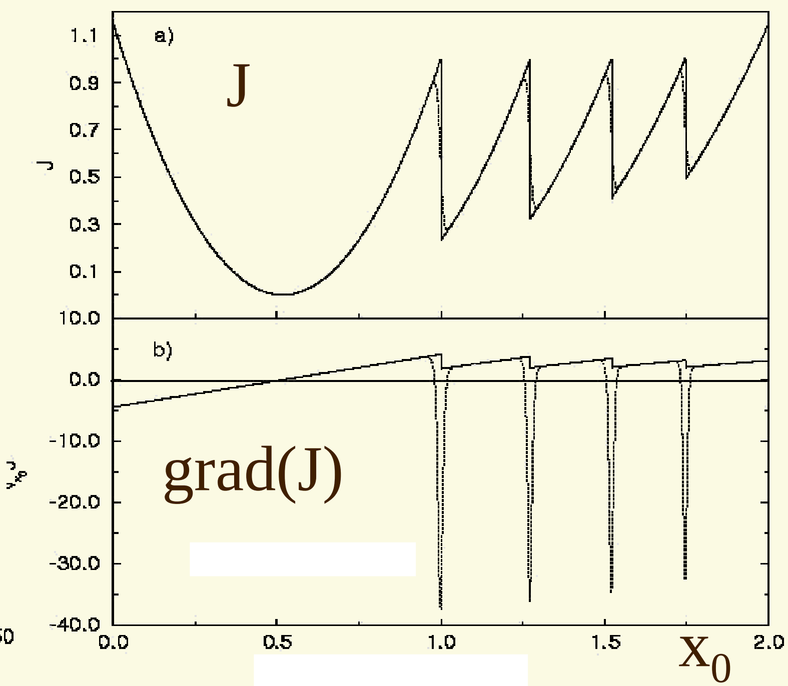
Smoothing the discontinuity

- ✓ Remove discontinuity in a simple model using smooth ftn.

$$\frac{\partial x}{\partial t} = \begin{cases} f_1(x), & x<x_c \\ f_2(x), & x\geq x_c \end{cases}$$

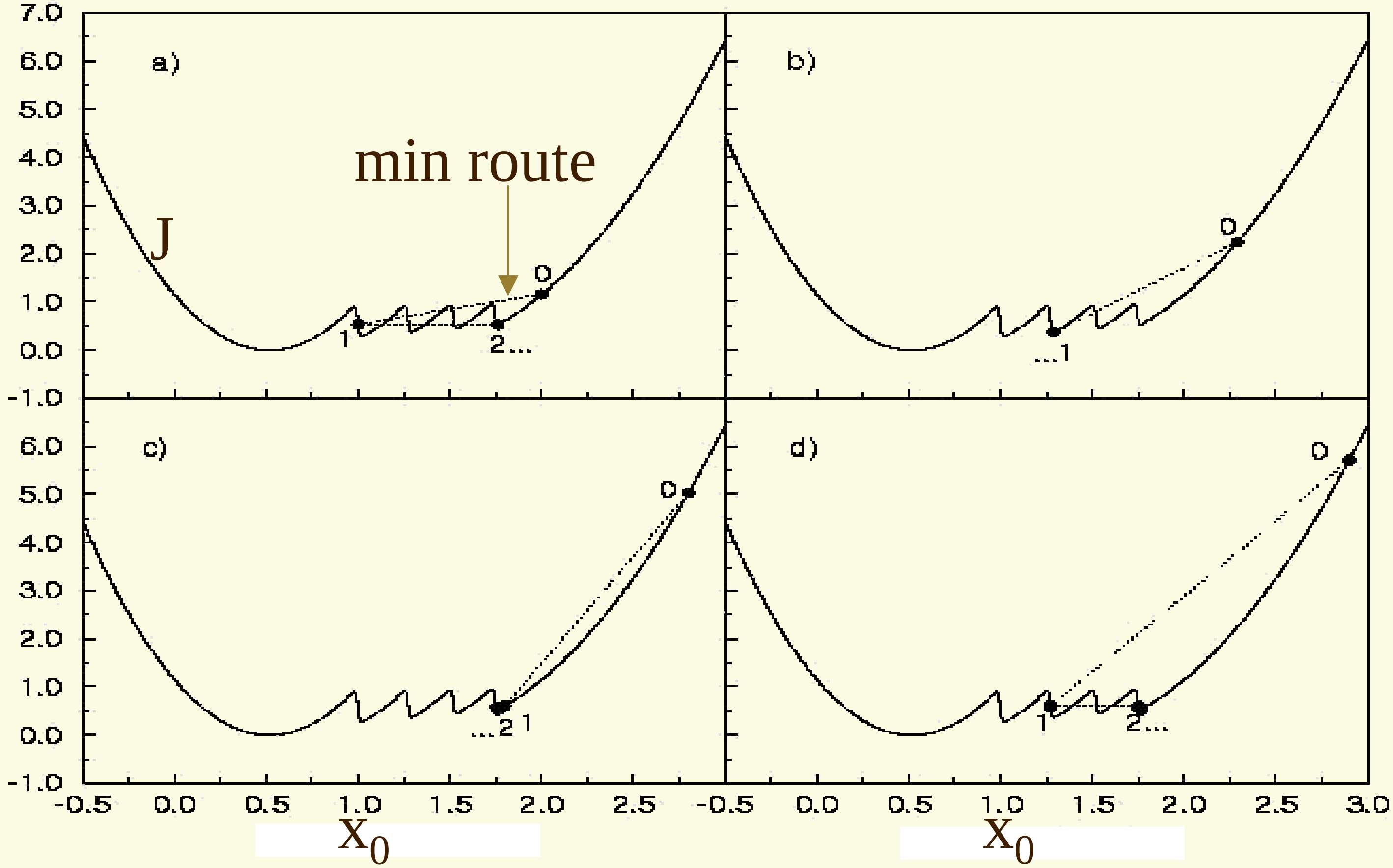
- ✓ Smoothing introduces extra stationary points for J.





Impact of smoothing: L-BFGS finds minimum in only 263 of 300, 37 failures.

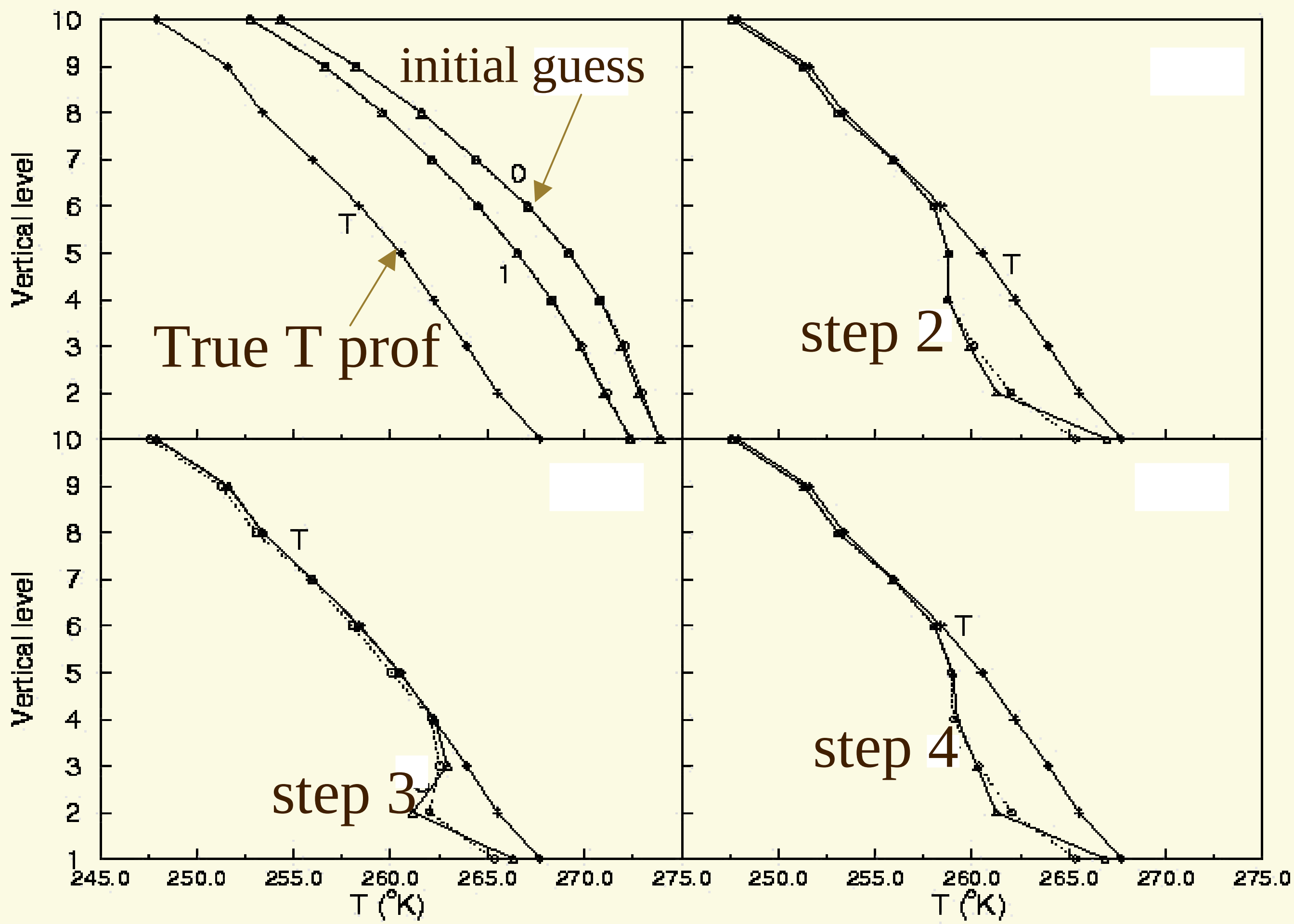
Same 4 ICs as in previous example:
Now trouble.



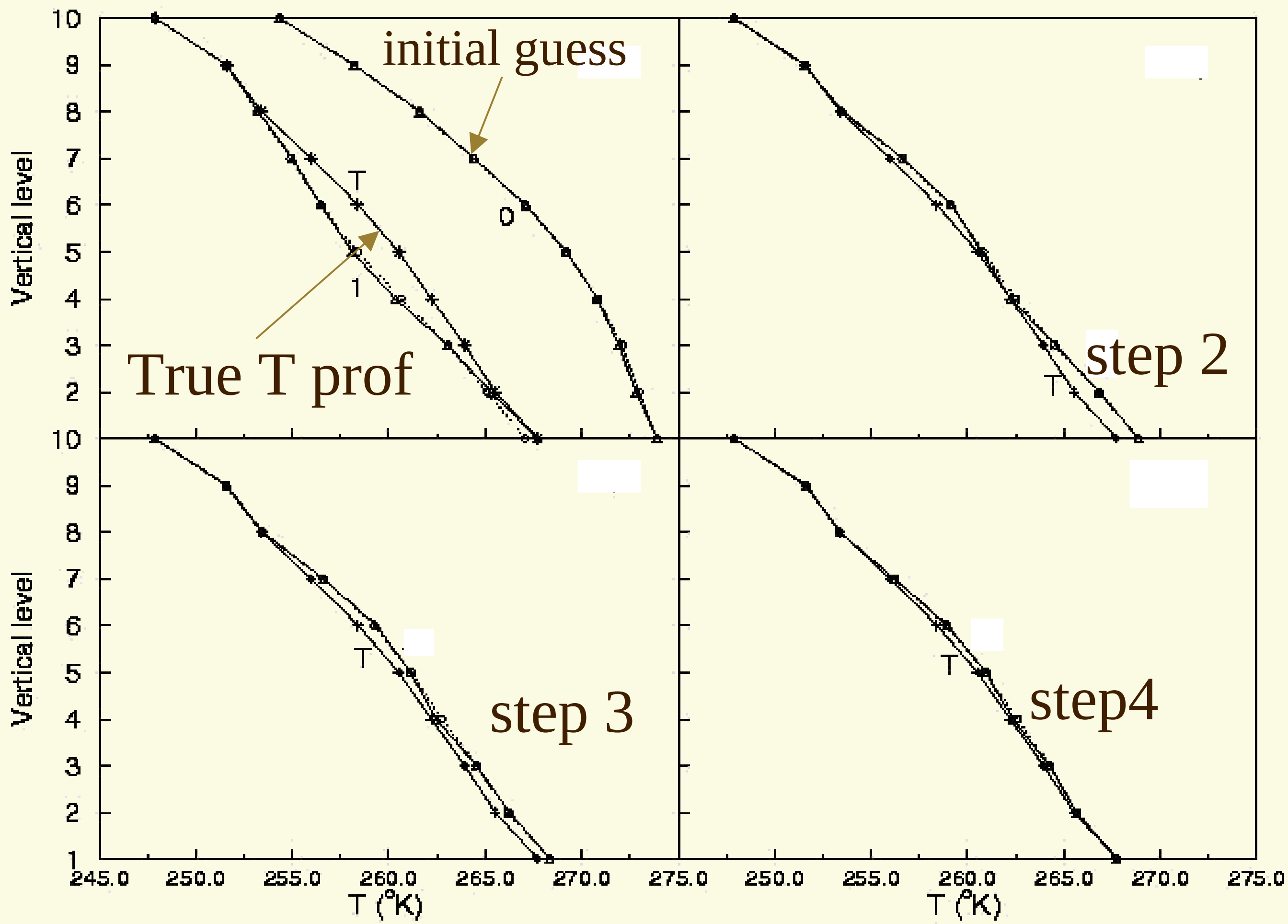
Can we do better? Test piecewise-differentiable "bundle" algorithm

- ✓ Test: $J = \sum w[f(\text{guess}) - f(\text{truth})]^2\}$
- ✓ Take f_i = shallow convection operator
  Discontinuities: conditional instability defines cloud base (lifting condensation level) and cloud top (highest instability level); different diffusion coefficients for different layers.
- ✓ Truth = T & q profiles for column 111 at 12N, 1 July 1995
- ✓ Initial guess = T & q profile for some other column at 12N or 12S. Try each column.
- ✓ Iterate to minimize J (to 0) using L-BFGS or bundle method
- ✓ Bundle method uses a bundle of gradients (side-grad) to construct a sub-gradient to force J to decrease.
- ✓ L-BFGS fails for 3 of 383 columns. Bundle method works for all, but computational cost almost double.

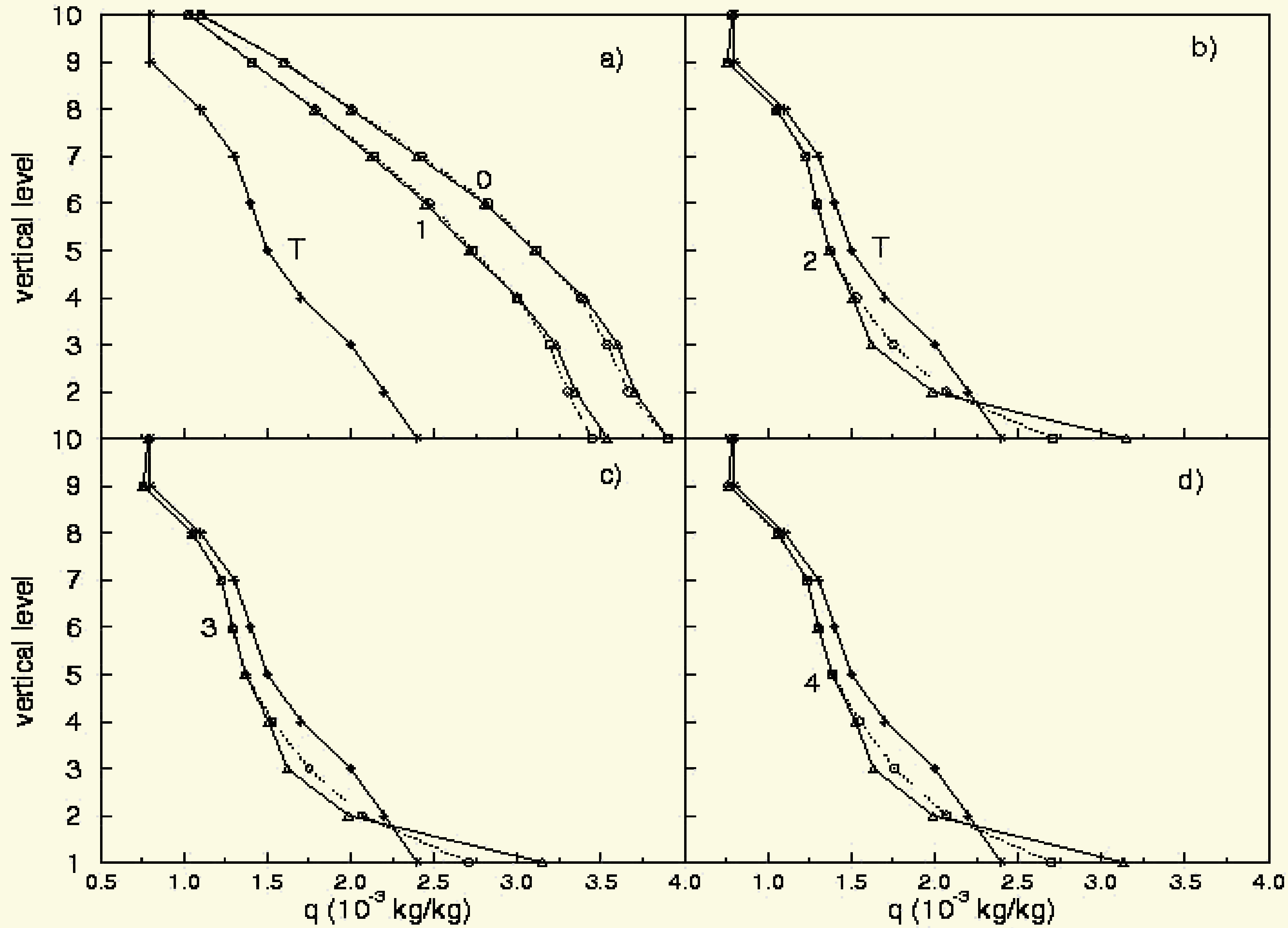
Tracing the route of minimization with L-BFGS for temperature profile



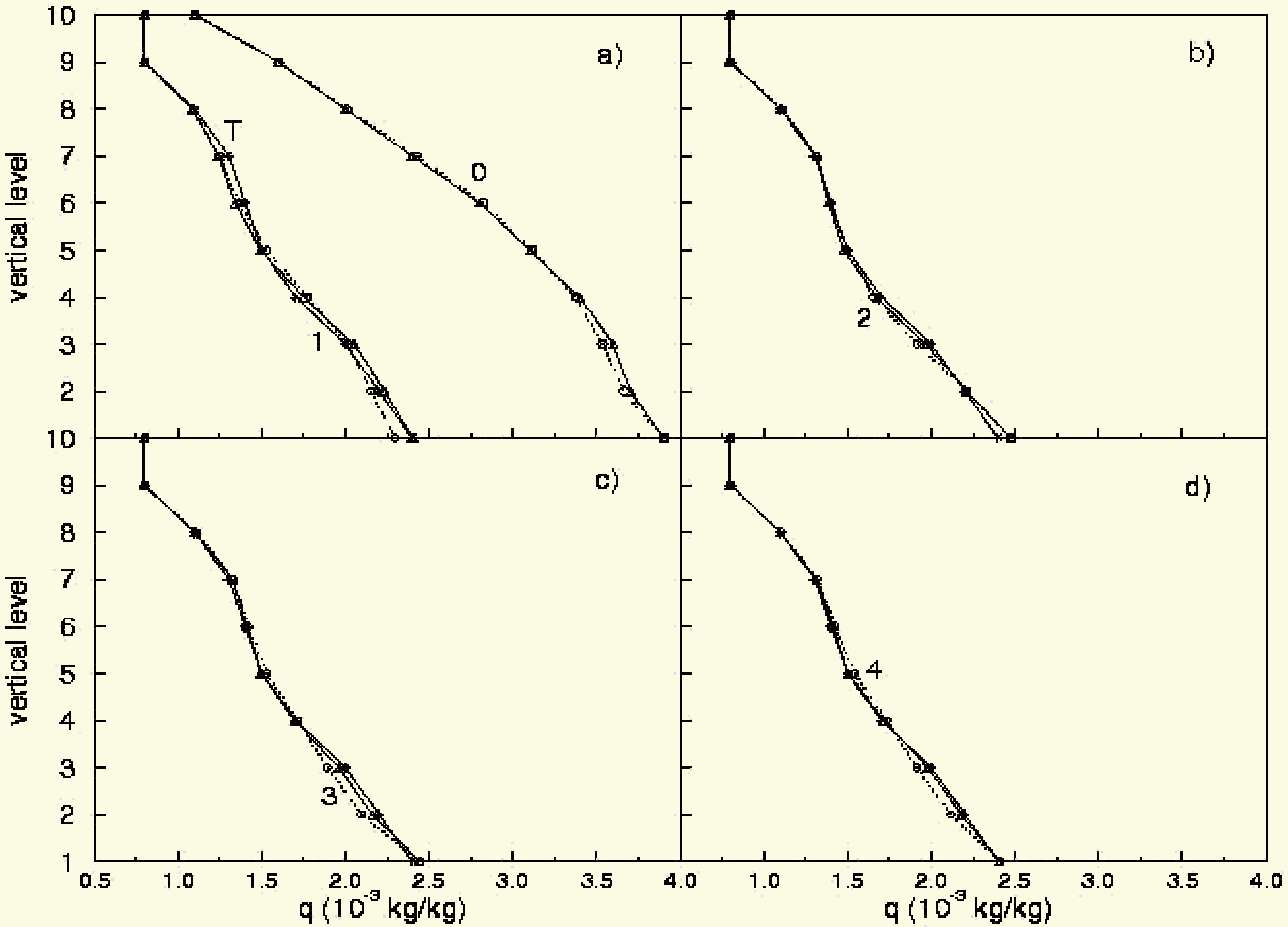
Tracing the route of minimization with bundle method for temperature profile



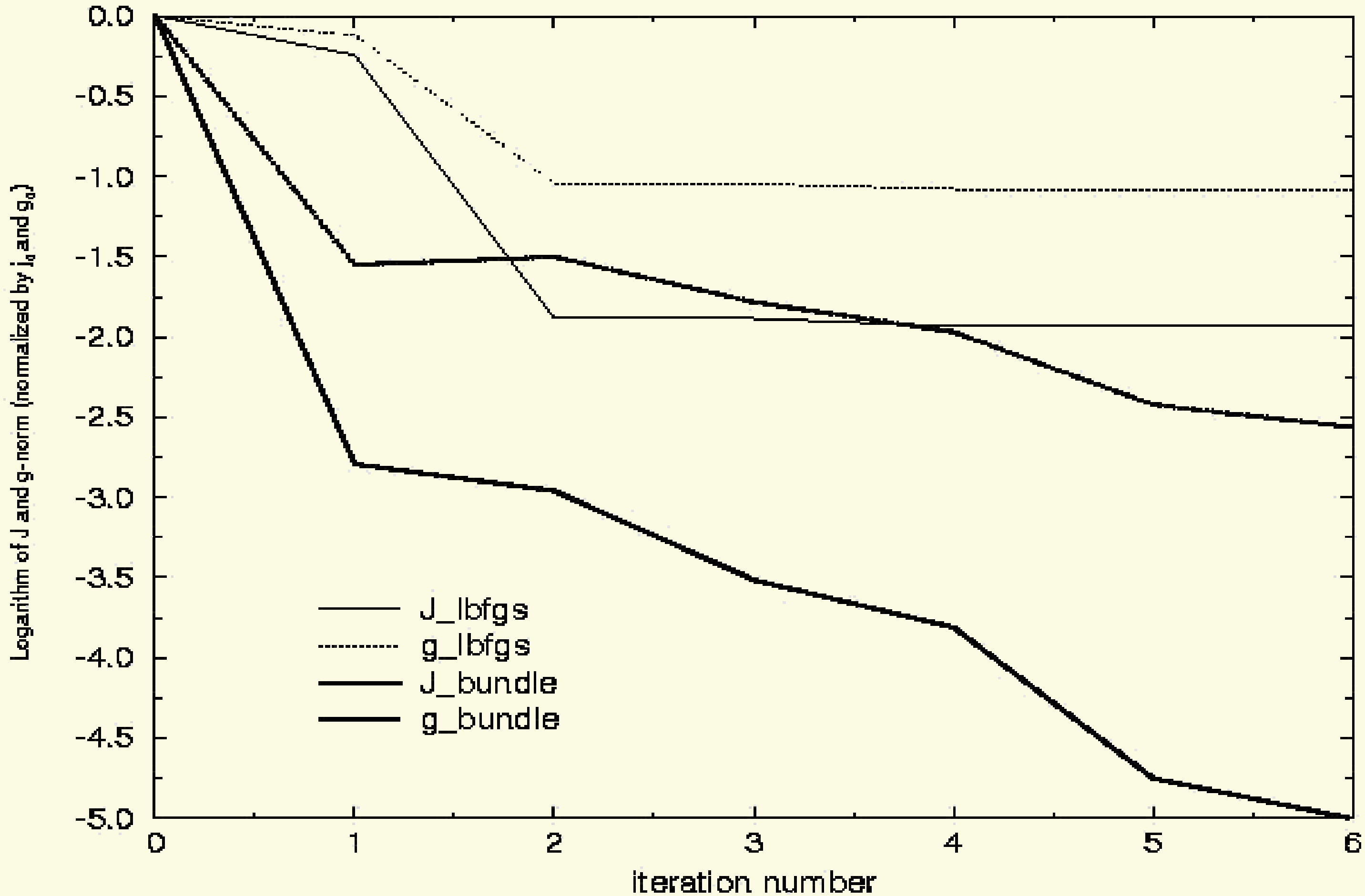
Tracing the route of minimization with L-BFGS for q profile



Tracing the route of minimization with bundle method for q profile

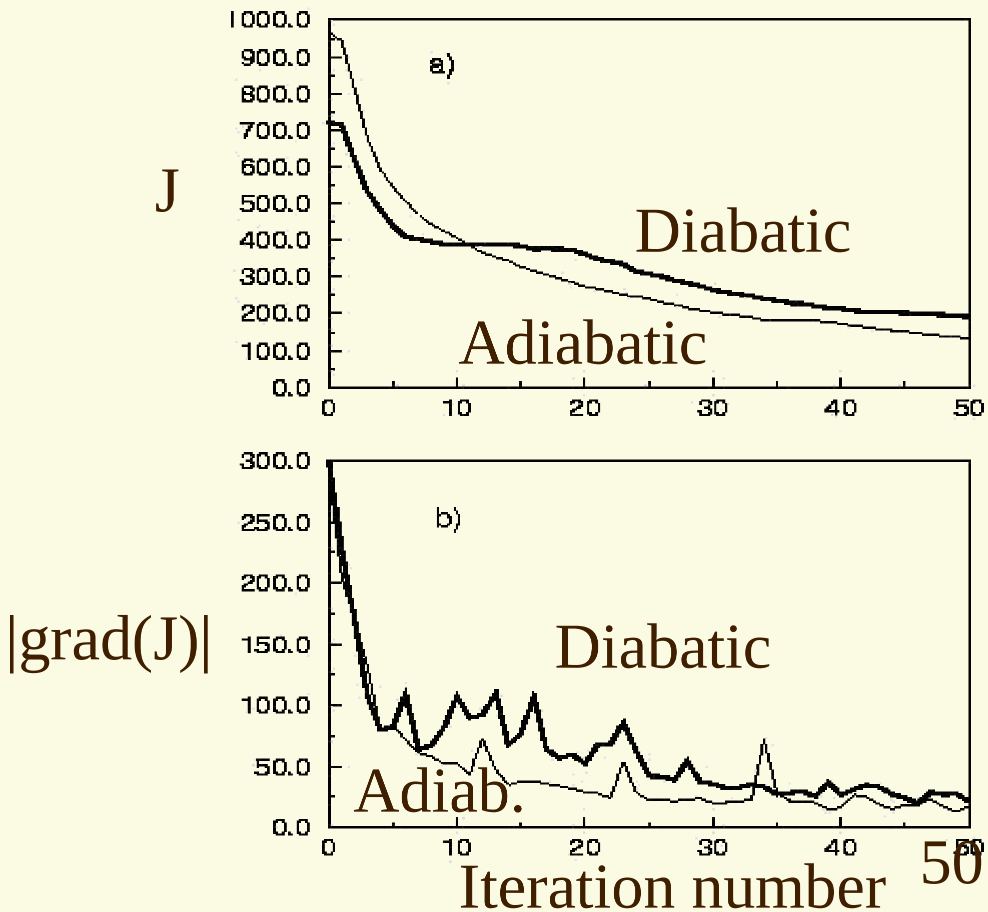


Decreases of J & ∇J for L-BFGS and bundle method

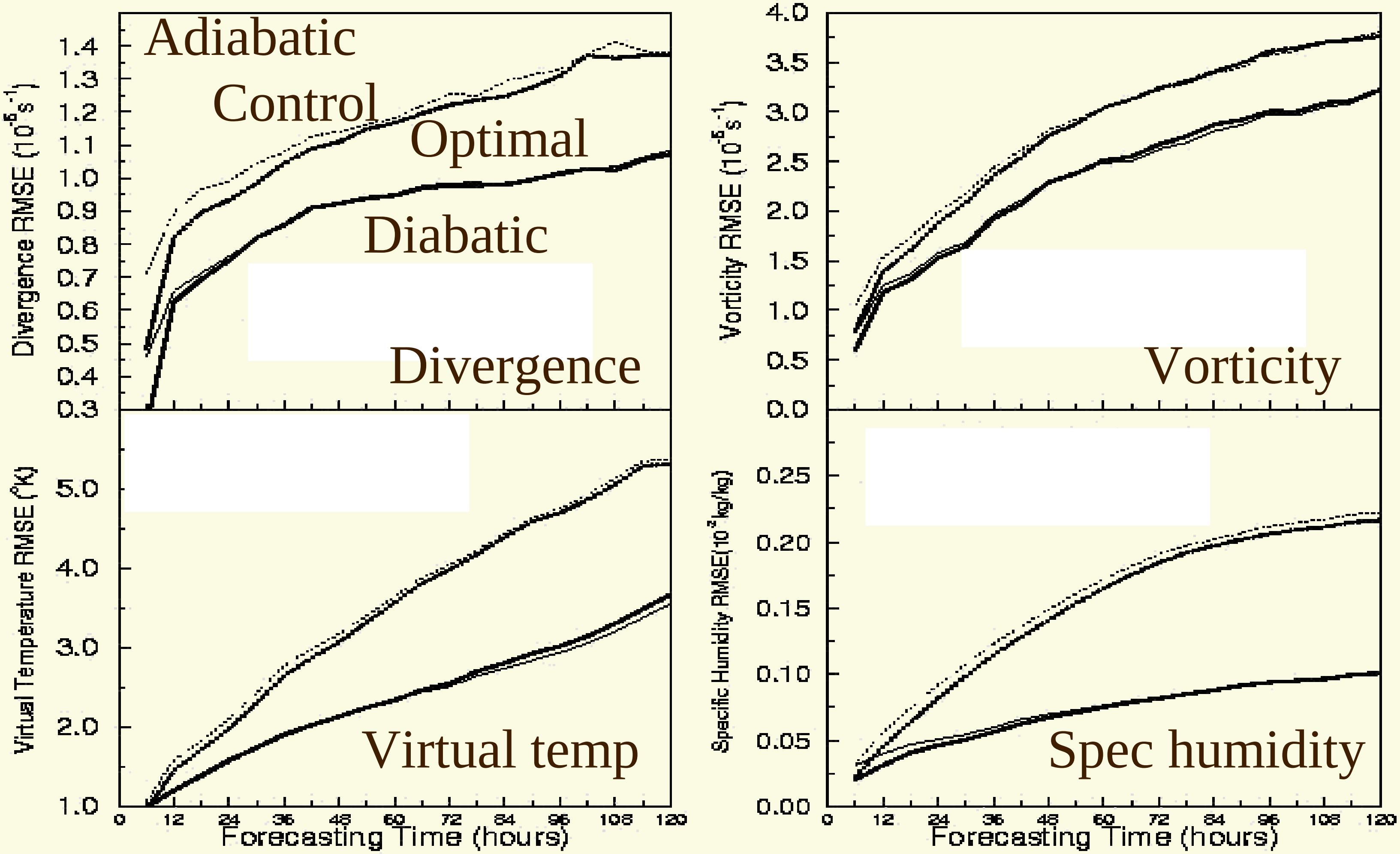


Performance of L-BFGS algorithm with ICs for NCEP global spectral model

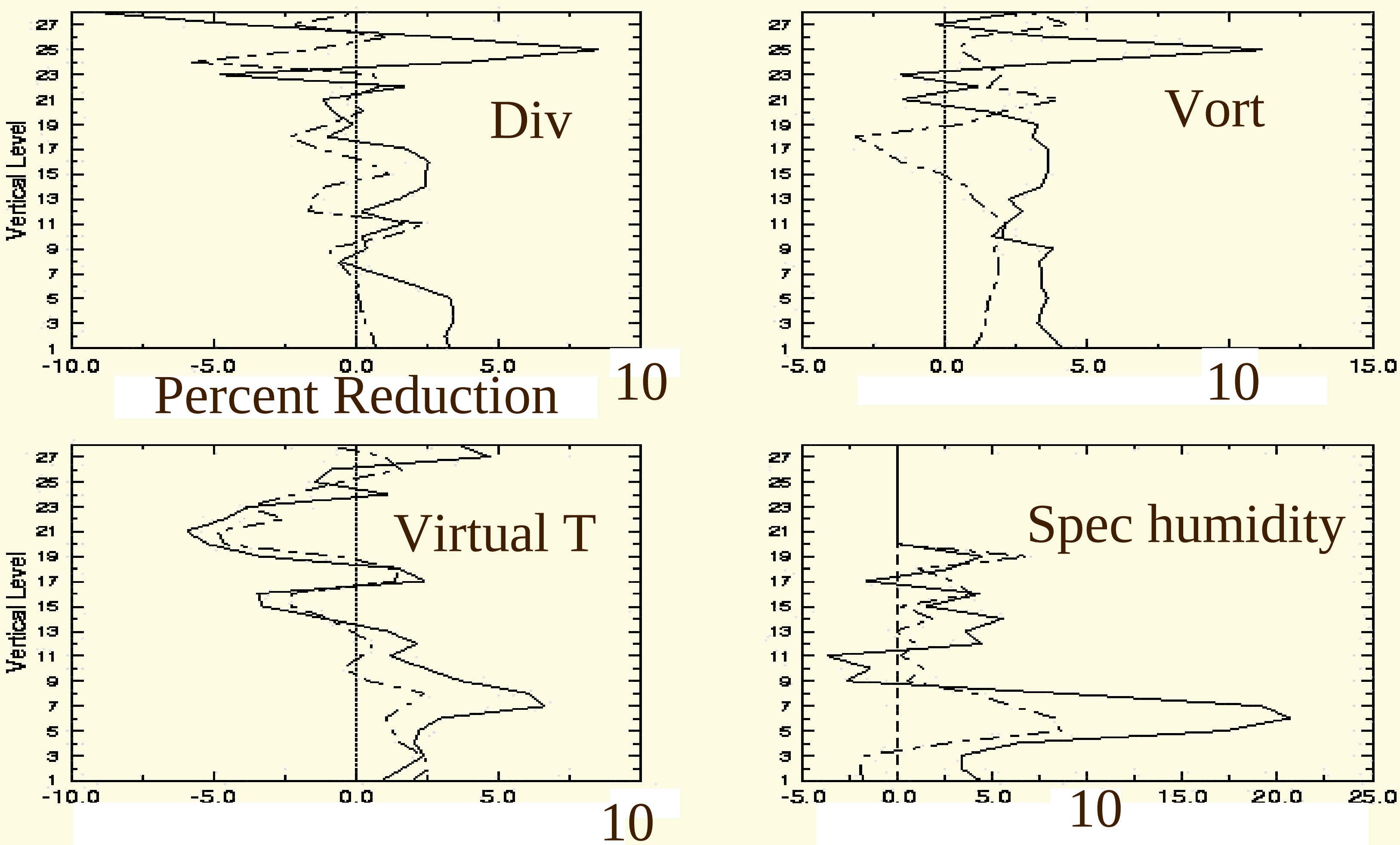
- ✓ Both discontinuity and nonlinearity introduced by parameterized physics affect decrease rate of J



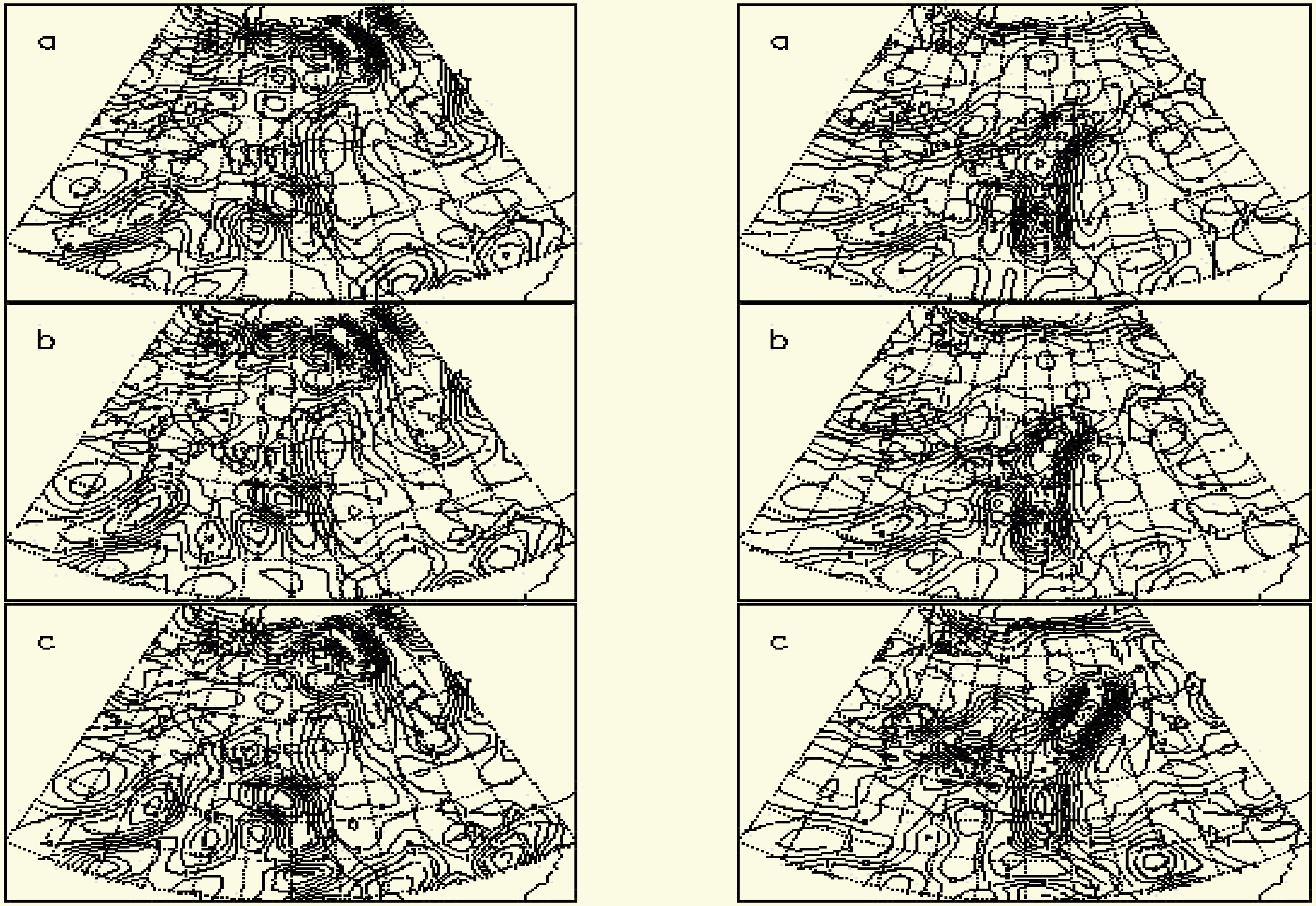
Change of RMSE with forecasting time (out to 5 days)



Vertical distribution of RMSE reduction at 24-h (solid line) & 48-h (dashed line)



Vorticity distribution at sigma=0.8838 over (0E,20N) to (60E,60N) at 6h & 30h forecasts



Summary: Can adjoint correctly evaluate grad(J) when physics are discontinuous?

- Cost function, J, of parameterized physics is piecewise differentiable. Max number of differentiable pieces is $k \cdot 2^n$ for k thresholds and n-step integration, so J becomes rough very fast with more thresholds and time steps.
- Perturbation analysis approach is invalid when a perturbation crosses a discontinuity.
- Adjoint integration is an implementation of the chain rule for differentiation of a complex model, which correctly evaluates gradients (or one-sided gradients) of a piecewise differentiable J.

Summary: Can Newton's method minimize discontinuous cost functions?

- ✓ L-BFGS method (Newton variant) often works well to minimize J, but stationary point may not be global minimum, and even sometimes fails.
- ✓ Bundle method better but twice as slow.

About 4D VAR:

- ✓ Optimal parameter values found by 4D VAR reduce forecast errors only out to 3 days.
  - Imperfect models: affect optimality of ICs and parameters for forecasts beyond optimization interval.
  - Uncertainty: intrinsic loss of predictability with increasing fcst leading time, particularly at small-scales.

Future Work: Classical 4D VAR

- ✓ Evaluate new physical parameterizations by checking cost function and its sensitivity.
- ✓ Test bundle method to minimize cost function for entire model.

My Future Work: Data assimilation for ensemble forecasting (Anderson '99)

- ✓ Given a set of observations, a Monte Carlo implementation of fully non-linear filter solves for a probability distribution of ICs, instead of seeking a single 'best' estimate of ICs.
- ✓ Extending the application to realistic model promises to enhance significantly the quality of ensemble forecasts over a range of spatial and temporal scales.
- ✓ Many obstacles need to be surmounted for the extension.

Thanks to

- ✓ Dr. Jon Ahlquist for his continuous scientific inspiration and many things more than science.
- ✓ My academic committee members: Drs. Barcilon, Navon, Pfeffer and Zou for their generous discussions and advice.
- ✓ Drs. Sela and Kalnay for their persistent encouragement and support.
- ✓ My wife and daughter for hope and love.
- ✓ My friends: Yin, Wei, K-Sris, Zhan, …
- ✓ All who gave me help and encouragement at FSU and NCEP

Questions?